TIME TABLE

(Registration on Monday at 8.30)

TIME	Monday	Tuesday	Wednesday	Thursday	Friday
	July 25	July 26	July 27	July 28	July 29
9.00 - 9.45	Troisi	Allen	Marchisio	Troisi	Reese
9.45 - 10.30	Troisi	Allen	Marchisio	Troisi	Reese
11.00 - 11.45	Allen	Carbone	Pagonabarraga	Allen	Marchisio
11.45 - 12.30	Allen	Carbone	Pagonabarraga	Allen	Marchisio
14.00 - 14.45	Troisi	Pagonabarraga	Reese	Carbone	
14.45 - 15.30	Troisi	Pagonabarraga	Reese	Carbone	
16.00 - 16.45	Carbone	Reese	Marchisio	Pagonabarraga	
16.45 - 17.30	Carbone	Reese	Marchisio	Pagonabarraga	

ADMISSION AND ACCOMMODATION

The registration fee is of 575,00 Euro + VAT taxes*, where applicable (bank charges are not included).

The registration fee includes a complimentary bag, four fixed menu buffet lunches (Friday subject to numbers), hot beverages, downloadable lecture notes and wi-fi internet access.

Applicants must apply at least one month before the beginning of the course. Application forms should be sent on-line through our web site: http://www.cism.it or by post.

A message of confirmation will be sent to accepted participants. If you need assistance for registration please contact our secretariat.

Applicants may cancel their course registration and receive a full refund by notifying CISM Secretariat in writing (by email) no later than two weeks prior to the start of the course.

If cancellation occurs less than two weeks prior to the start of the course, a Euro 50,00 handling fee will be charged. Incorrect payments are subject to Euro 50,00 handling fee.

A limited number of participants from universities and research centres who are not supported by their own institutions can be offered board and/or lodging in a reasonably priced hotel or students' dormitories, if available.

Requests should be sent to CISM Secretariat by **May 25, 2016** along with the applicant's curriculum and a letter of recommendation by the head of the department or a supervisor confirming that the institute cannot provide funding. Preference will be given to applicants from countries that sponsor CISM.

Information about travel and accommodation is available on our web site, or can be mailed upon request.

* Italian VAT is 22%.

For further information please contact:

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Piazza Garibaldi 18
33100 Udine (Italy)
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ACADEMIC YEAR 2016

The Leipholtz Session

Centre International des Sciences Mécaniques
International Centre for Mechanical Sciences

MULTISCALE MODELING OF FLOWING SOFT MATTER AND POLYMER SYSTEMS

Advanced School
coordinated by

Paola Carbone
University of Manchester
UK

Daniele Marchisio
Politecnico di Torino
Italy

Udine ***July 25 - 29*** 2016

MULTISCALE MODELING OF FLOWING SOFT MATTER AND POLYMER SYSTEMS

Soft materials such as **polymer melts** or solutions, **colloidal suspensions, emulsions, foams** and **gels** are materials lying at the interface between fluids and solids requiring, for their simulation, highly innovative computational methods. In a similar way, simulation of fluid flows in nanoscale geometries also needs to account for the molecular nature of the fluid while at the same time retrieving hydrodynamic properties.
This advanced school aims at covering the theory and practice of multiscale modeling of these materials (and the corresponding chemical processes involved) and is specifically **addressed to graduate students in physics, chemistry and engineering** (chemical, mechanical, environmental, computational) and to scientists and engineers already working in the field.
Particular attention will be paid to full-atom and coarse-grained molecular dynamics, dissipative particle dynamics, hybrid molecular/continuum methods, and computational fluid dynamics.
Some lectures will focus on **molecular dynamics**, which is currently used for the estimation of equilibrium (thermodynamic) and non-equilibrium (transport) properties of complex systems. These simulations can employ models with all the structural details of the chemical system (called **full-atom**) or with only few of them (known as coarse-grained models). Molecular Dynamics treats the atoms as classical objects following Newtonian dynamics, but relies on information obtained from quantum chemistry, which will be also covered in this advanced school. Force fields (employed in molecular dynamics) and many other important properties (such as partial/net atomic charges) are often derived from **quantum chemistry** calculations, which are also useful for the estimation of chemical reaction rates.
As the chemical complexity of the new materials increases it becomes necessary to develop rapid methods to parametrize reasonably accurate atomistic force fields. In selected applications, e.g. soft materials for electronics, the microstructure and dynamics of the material influences its electronic structure, i.e. one needs larger scale simulations to understand smaller scale properties.
With these modeling techniques, the size of the simulated systems is very limited; the simulation of larger systems requires the use of further coarse-graining, or hybrid methods, that link molecular to hydrodynamic models. Among the different techniques available at these larger time- and length-scales, **dissipative particle dynamics**, certain **hybrid methods**, and **computational fluid dynamics** will be covered. Some lectures will describe the extension of these methods to the simulation of multiphase systems and will discuss some of the numerical issues related to the solution of the governing equations with the finite volume method. Finally, some applications related to the simulation of polymer self-assembly in solution and polymer foam expansion and evolution will be described.

PRELIMINARY SUGGESTED READINGS

Allen M.P. , Tildesley D.J., Computer Simulation of Liquids (Oxford University Press, 1989).

Betz R.M., Walker R.C., J. Comp. Chem. 36, 79-87 (2015).

Borg M.K., Lockerby D.A., Reese J.M. J. Fluid Mech. 768, 388-414 (2015).

Dongari N., Zhang Y.H., Reese J.M. J. Phys. D: Appl. Phys, 44, 125502 (2011).

Frenkel D., Smit B., Understanding Molecular Simulation (Academic Press, 2001).

Karimi-Varzaneh H.A., Van Der Vegt N.F.A., Muller-Plathe F., Carbone P., ChemPhysChem, 13, 3428-3439 (2012).

Lockerby D.A., Duque-Daza C.A., Borg M.K., Reese J.M., J. Comp. Phys. 237, 344-365 (2013).

Lockerby D.A., Patronis A., Borg M.K., Reese J.M, J. Comp. Phys. 284, 261-272 (2015).

Marchisio D.L., Fox R.O., Computational models for polydisperse particulate and multiphase systems (Cambridge University Press, 2013).

Noid W.G., J. Chem. Phys. 139, 090901 (2013).

Wang L.-P., Chen J., Van Voorhis T., J. Chem. Theor. Comput. 9, 452-460 (2013).

Wang L.-P., Martinez T. J., Pande V. S., J. Phys. Chem. Lett. 5, 1885-1891 (2014).

LECTURES

All lectures will be given in English. Lecture notes can be downloaded from the CISM web site, instructions will be sent to accepted participants.

INVITED LECTURERS

Michael Allen - University of Bristol, UK
6 lectures on: Full-atom molecular dynamics.
Theoretical background: basic statistical mechanics, static and dynamical properties. Methodology: periodic boundary conditions, the MD algorithm, forcefields. Applications: sampling different ensembles, thermostats and barostats, molecular dynamics of fluid flow and nonequilibrium behaviour.

Paola Carbone - University of Manchester, UK
6 lectures on: Coarse-grained molecular dynamics.
Theoretical background/methodology: scalability of the molecular dynamics algorithm, methods of reducing degrees of freedom in a molecular model (bottom-up and top-down approaches). Systematic coarse-graining: structural and thermodynamic techniques), how to tune the degree of coarse-graining and develop atomistic and coarse-grained models Applications: modeling of soft matter (polymers and surfactants) and simple solutions.

Daniele Marchisio - Politecnico di Torino, Italy
6 lectures on: Continuum modeling of single phase and multiphase flows.
Theoretical background: link between the molecular and the continuum descriptions: Liouville, Boltzmann and Navier-Stokes equations. Methodology: numerical and computational aspects (finite-volume method). Applications: Simulation of multiphase, soft and polymer systems.

Ignacio Pagonabarraga - Universitat de Barcelona, Spain
6 lectures on: Dissipative particle dynamics.
Theoretical background/methodology: mesoscopic simulations of heterogeneous materials and their applications on complex fluids. Formulation of thermodynamically consistent mesoscopic models with appropriate hydrodynamic behaviour. Relationship between dissipative particle dynamics and other coarse grained, hydrodynamically consistent particle-based methods.

Jason Reese - University of Edinburgh, UK
6 lectures on: Continuum / multiscale modeling of fluids.
Hybrid particle/fluid solvers: domain-decomposition vs heterogeneous methods, sequential vs concurrent methods. Coupling methods for time advancement of multiscale dynamic systems. Higher-order hydrodynamic approaches for gas flows. Engineering applications: micro-jet actuators, water flowing carbon nanotubes, thermally-driven gases, etc.

Alessandro Troisi - University of Warwick, Coventry, UK
6 lectures on: Quantum chemistry for and from classical simulations.
One-electron approximation, variational principle and basis sets, Hartree Fock and DFT methods. Computable properties. Procedures to generate classical force fields from electronic structure calculations. Force matching approaches. Application to organic electronics.

MULTISCALE MODELLING OF FLOWING SOFT MATTER AND POLYMER SYSTEMS

Udine, July 25 - 29, 2016
Application Form
(Please print or type)

Surname _____

Name _____

Affiliation_____

Address_____

_____

E-mail _____

Phone _____Fax_____

Method of payment upon receipt of confirmation (Please check the box)

The fee is 575,00 Euro + 22% Italian VAT taxes, where applicable (bank charges are not included).

❑ *I shall send a check of Euro* _____

❑ *Payment will be made to CISM - Bank Account No. 094570210900, VENETO BANCA - Udine (CAB 12300 - ABI 05035 - SWIFT/BIC VEBHIT2M - IBAN CODE IT46 N 05035 12300 09457 0210900). Copy of the receipt should be sent to the secretariat*

❑ I *shall pay at the registration counter with check or VISA Credit Card (Mastercard/Eurocard, Visa, CartaSi)*

IMPORTANT: CISM is obliged to present an invoice for the above sum. Please indicate to whom the invoice should be addressed.

Name _____

Address _____

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C.F.* _____

VAT/IVA* No _____

(*) Only for EU residents or foreigners with a permanent business activity in Italy.

Only for Italian Public Companies

❑ *I ask for IVA exemption (ex law n. 537/1993 - art. 14 comma 10).*

Privacy policy: I understand that data received via this form will be used only to provide information about CISM and its activities, within the limits set by the Italian legislative decree no. 196/2003 and subsequent amendments.
Complete information on CISM's privacy policy is available at www.cism.it.

I have read the "Admission and Accommodation" terms and conditions and agree.

Date _____ Signature _____